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LETTER TO THE EDITOR

The quantum theory for anomalous low-temperature thermal conductivity of non-crystalline dielectric solids

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Abstract. We discuss the interaction between two-level systems and the phonon field in non-crystalline dielectric solids, and we calculate the quantum transition matrix elements of such an interaction. After studying the Boltzmann equation for phonon transport, we obtain the phonon distribution function. From a direct calculation of the heat current, and as a result of obtaining the thermal conductivity of non-crystalline dielectric solids, the T^2 relation is obtained.

It has been shown that the thermal conductivity of non-crystalline dielectric solids is far lower than that of crystalline solids and has a special T^2 temperature dependence [1–3]. Almost simultaneously Anderson [4] and Phillips [5] put forward a model based on a two-level system. They assumed that a certain number of atoms have two equilibrium positions in an asymmetric double-well potential, and that transitions between the two positions are possible via tunnelling, whereby a resonant phonon is absorbed or emitted. They gave an explanation of the anomalous low-temperature thermal conductivity of non-crystalline dielectric solids and obtained a T^2 temperature dependence. However, in their work a relaxation time approximation is used and the relaxation time is calculated using a quasi-classical method like that used by Einstein to discuss the interaction between atoms and a radiation field. In this letter, this problem has been considered by avoiding the relaxation time approximation and using the Boltzmann equation and quantum transition theory only.

The derivation of the T^2 dependence of the thermal conductivity (for temperatures less than 1 K is described as follows. Heat current is carried by phonons in non-crystalline dielectric solids, and the Boltzmann equation has the form

$$\partial n / \partial t + v_{\lambda} \cdot \nabla_{\lambda} n = C_{(n)} \quad (1)$$

where n is the density distribution of the phonon gas, v_{λ} is the group velocity of a phonon. $C_{(n)}$ is the collision term and λ is phonon label. The collision term contains 'normal' processes, 'Umklapp' processes, scattering between phonons and two-level systems, boundary scattering and other scattering. 'Normal' processes and 'Umklapp' processes are interactions between phonons and they can be omitted at low temperatures. We also omit the boundary scattering and other scattering. Therefore, only the interactions between phonons and two-level systems are left.

The density distribution of the phonon gas depends on temperature only through $\nabla_r T$ in the steady state, i.e.

$$v_\lambda \cdot \nabla_r T \, dn/dT = C_1 \quad (2)$$

where C_1 are the interactions between phonons and two-level systems. According to the Boltzmann distribution law, the probability of a two-level system staying in its ground state is A_1 and the probability of the two-level system staying in an excited state is A_2 , so

$$A_1 = 1/(1 + e^{-E/k_B T}) \quad (3)$$

$$A_2 = 1/(1 + e^{E/k_B T}) \quad (4)$$

where E is the energy difference between the ground state and the excited state. The interaction Hamiltonian between two-level systems and the phonon field has the form

$$H = \frac{1}{2} \begin{pmatrix} D & 2M \\ 2M & -D \end{pmatrix} \sum_k \sqrt{\frac{\hbar k}{2\rho V v}} (a_k - a_k^\dagger) \quad (5)$$

where D and M are coupling constants between two-level systems and the phonon field, k is the absolute value of the wave vector, ρ is the mass density, V is the volume of the non-crystalline dielectric solid and v is the group velocity of the low-frequency phonons. Accompanying the transition from the ground state to the excited state of the two-level system, one phonon with frequency ω is destroyed. The transition probability has the form

$$P_1 = (2\pi/\hbar) M^2 n (\hbar k / 2\rho V v) \delta(E - \hbar\omega) \quad (6)$$

where n is the phonon number. Conversely, for the transition from the excited state to the ground state, one phonon with frequency ω is created and the transition probability has the form

$$P_2 = (2\pi/\hbar) M^2 (n + 1) (\hbar k / 2\rho V v) \delta(E - \hbar\omega). \quad (7)$$

The collision term has the form

$$C_1 = \int P_2 A_2 P(E') \, dE' \, dV' - \int P_1 A_1 P(E') \, dE' \, dV' \quad (8)$$

where $P(E)$ is the density of states of two-level systems in unit volume. Through concrete calculation, we obtain the following form

$$C_1 = (\pi M^2 k P(E) / \rho v) \left((n + 1) / (1 + e^{E/k_B T}) - n / (1 + e^{-E/k_B T}) \right). \quad (9)$$

We define

$$n = n_0 + n_1 \quad (10)$$

where n_0 is the phonon number at thermal equilibrium. According to Planck's law

$$n_0 = 1 / (e^{E/k_B T} - 1). \quad (11)$$

Under conditions of thermal equilibrium, n equals n_0 and the collision term is zero,

so

$$C_1 = (\pi M^2 k P(E) / \rho v) [1 / (1 + e^{E/k_B T})] - [1 / (1 + e^{-E/k_B T})] n_1. \quad (12)$$

The contribution of the n_0 term is retained when considering dn/dT , so

$$dn/dT \approx (e^{E/k_B T} / (e^{E/k_B T} - 1)^2) \hbar \omega / k_B T^2. \quad (13)$$

Substituting (12) and (13) into (2), we obtain

$$n_1 = [e^{E/k_B T} / (e^{E/k_B T} - 1)^2] (\hbar \omega / k_B T^2) v_\lambda \cdot \nabla_r T \{ (\pi M^2 k P(E) / \rho v) \\ \times [1 / (1 + e^{E/k_B T}) - 1 / (1 + e^{-E/k_B T})] \}^{-1}. \quad (14)$$

The heat current in unit volume has the form

$$Q = (1/V) \sum_\lambda n(\lambda) \hbar \omega_\lambda v_\lambda \quad (15)$$

where v_λ is the group velocity of a phonon. n_0 has no contribution to the heat current, so

$$Q = (1/V) \sum_\lambda n_1(\lambda) \hbar \omega_\lambda v_\lambda. \quad (16)$$

Regarding non-crystalline dielectric solids as isotropic materials, Q has the form

$$Q = -k \nabla T. \quad (17)$$

With a temperature gradient in the x direction alone, we obtain

$$n_1 = [e^{E/k_B T} / (e^{E/k_B T} - 1)^2] (\hbar \omega / k_B T^2) v_{\lambda x} (dT/dx) \{ (\pi M^2 k P(E) / \rho v) \\ \times [1 / (1 + e^{E/k_B T}) - 1 / (1 + e^{-E/k_B T})] \}^{-1}. \quad (18)$$

Substituting (18) and (16) and contrasting this with (17), we obtain

$$n = \frac{1}{V} \sum_\lambda \frac{e^{E/k_B T}}{(e^{E/k_B T} - 1)^2} \frac{\hbar^2 \omega^2}{k_B T^2} v_{\lambda x}^2 \left[\frac{\pi M^2 k P(E)}{\rho v} \left(\frac{1}{1 + e^{-E/k_B T}} - \frac{1}{1 + e^{E/k_B T}} \right) \right]^{-1}. \quad (19)$$

For low frequencies in a non-crystalline dielectric solid, the density of states of phonons has the Debye form

$$g(\omega) = (V/2\pi^2) \omega^2 / v^3 \quad (20)$$

and the dispersion relation has the form

$$\omega = kv. \quad (21)$$

Low-frequency terms play an important role in equation (19) (we omit the high-frequency terms). $P(E)$ should be non-zero and continuous in the vicinity of $E = 0$, and we use the approximation $P(E) = P_0$. Replacing the summation by an integration from

0 to ∞ , equation (19) can be expressed as

$$k = \frac{1}{V} \int_0^\infty d\omega \frac{V}{2\pi^2} \frac{\omega^2}{v^3} \frac{e^{E/k_B T}}{(e^{E/k_B T} - 1)^2} \frac{\hbar^2 \omega^2}{k_B T^2} v_x^2 \times \left[\frac{\pi M^2 \omega P_0}{\rho v^2} \left(\frac{1}{1 + e^{-E/k_B T}} - \frac{1}{1 + e^{E/k_B T}} \right) \right]^{-1}. \quad (22)$$

Assuming $\hbar\omega/k_B T = y$, we can get

$$k = \frac{k_B^3 \rho}{2\pi^3 \hbar^2 M^2 P_0} T^2 \int_0^\infty dy \frac{v_x^2}{v} \frac{e^y}{(e^y - 1)^2} y^3 \left[\frac{1}{1 + e^{-y}} - \frac{1}{1 + e^y} \right]^{-1}. \quad (23)$$

v_x^2/v depends on the characteristics of the material. ρ , M and P_0 are physical quantities describing characteristics of non-crystalline materials. The integration can also be calculated. We have calculated the quantum transition matrix element and from the Boltzmann equation of phonon transport, we get the phonon distribution function. Finally, we get the T^2 relation of the thermal conductivity of non-crystalline dielectric solids. Considering the isotropy condition, v is regarded as a constant and, assuming $v_x^2 = (1/3)v^2$, we get

$$k = \frac{k_B^3 \rho v}{6\pi^3 \hbar^2 M^2 P_0} T^2 \int_0^\infty dy \frac{e^y}{(e^y - 1)^2} y^3 \left[\frac{1}{1 + e^{-y}} - \frac{1}{1 + e^y} \right]^{-1}. \quad (24)$$

Performing the integration, the final form is obtained:

$$k = 9.87(k_B^3 \rho v / 6\pi^3 \hbar^2 M^2 P_0) T^2. \quad (25)$$

In conclusion, in this letter, the relaxation-time approximation and the quasi-classical method for calculating the relaxation time are avoided. The physical process is therefore more direct and the physical model is more basic. However, we should recognize that this work is based on the phenomenological theory for a two-level system. A microscopic theory with universal significance is required to explain the problem in more detail and more satisfactorily.

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